Mechanical Properties and Evidence of Asymmetrical X-Ray Diffraction Peak Broadening in Crystalline $Ge_2Sb_2Te_5$ Thin Films

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Te-based chalcogenides materials gathered a high interest because of their increasingly important role in the technological applications. Indeed, in the last decades they have been adopted in non-volatile memory devices as replacement of traditional charge trap technologies [1-3]. Phase-Change Memory or "PCM" technology bases its functionality on the reversible phase transition of a chalcogenide alloys between an amorphous and a crystalline phase, induced by an electrical pulse, leading to a huge change of the electrical resistivity into the device. This allows storing two or more "bits" in a single memory cell [4]. Among all the different types of emerging memory technologies, PCM was the first one to reach the volume production proving its already high maturity. Furthermore, PCM recently achieved the highest level of reliability (i.e. grade 0), demonstrating its suitability for the embedded automotive market [4-5].

A wide variety of phase-change materials have been already studied, however $Ge_2Sb_2Te_5$ (GST) remains the most studied material because of its congruent nature and its key role in more complex alloys [6]. Prototypical GST presents a stable stoichiometry, without atoms diffusion or phase segregation during the amorphous to crystalline phase transition. Under thermal annealing, amorphous GST first crystallizes into a face-centered cubic (f.c.c.) phase (space group: Fm-3m). During this phase transition, a density increase and a thickness reduction have been observed in several references [8-8]. This volume shrinking results in the build-up of a significant tensile stress.

XRD is the best-suited characterization technique to investigate strain and microstrain by a microstructural point of view. Complementary to TEM, XRD give an average characterization on a large sample volume with relevant grain statistics and has a very high resolution in the reciprocal lattice. Sensitive strain effects are the observable on X-ray diffraction (XRD) patterns, such as peaks shifts (macroscopic strain) and peaks broadening (microscopic strain).
More generally, X-ray diffraction peaks broaden when the crystal lattice becomes imperfect. According to the theory of kinematical scattering, peaks broadening, characterized by the Full Width Half Maximum (FWHM) of the diffraction peaks, originates from small crystallites size effects and/or if lattice defects (heterogeneity, microstrain, gradient) are present in enough large abundance.

Extensive studies have already been conducted on chalcogenide materials using XRD, however full, consistent, fine and deep studies of line profiles in crystalline f.c.c. GST films has not yet been reported.

In this work and for the first time, thermally crystallized f.c.c. GST thin films are studied by X-ray diffraction through multi-{hkl} reflection, at different tilt directions of the film (**Fig. 1**) and focused on peaks positions and line profiles broadening.
Consistent, full and deep investigations are carried out, to give new insight on the mechanical state of crystalline cubic $Ge_2Sb_2Te_5$. This full large Reciprocal Space Mapping and deep data analysis allow to deduced the X-Ray Elastic Constant (XEC). In addition and as special focus, an atypical asymmetric line profile broadening (or peak shape) of Bragg peaks is also observed and discussed, with the support of instrumental and material considerations.

References

1. F. Arnaud et al., IEDM, 2018,18.4.1-4.
2. M. Le Gallo et al. 2020 J. Phys. D: Appl. Phys., 2020, 53 213002.
3. P. Noe, et al., Semicond, Sci. & Tech., 2018, 33, 013002.
4. A. Athmanathan et al., IEEE J. on Emerging and Selected Topics in Circuits and Systems, 2016, 6, 1, 87.
5. P. Cappelletti et al 2020 J. Phys. D: Appl. Phys., 2020, 53 193002.
6. L. Prazakova et al., Materialia, 21, 2022, 101345.
7. F. Fillot et al. J. of Appl. Cryst., 51, 2018, 1991.
8. Q. Zhang et al., AIP Advances, 2023, 13, 015014.

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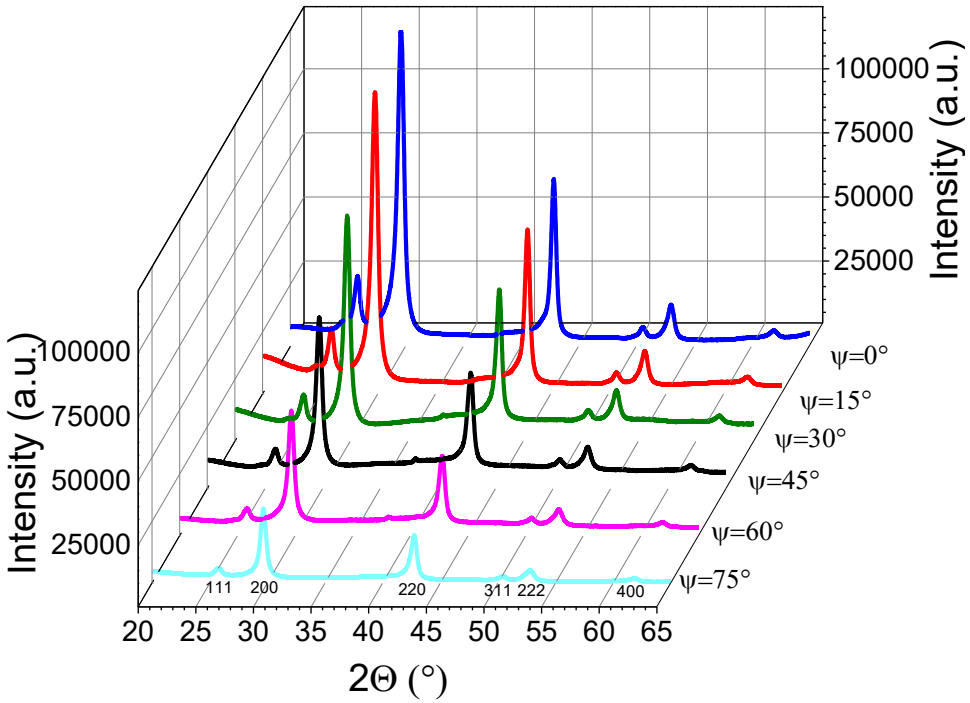

Fig. 1: θ-2θ scans at different tilt angle (Ψ) for the thermally crystallized GST sample. The {hkl} reflections are indexed and correspond to the f.c.c. GST phase. All the same {hkl} reflections are observable at the different Ψ angles. By fitting the Bragg peaks, 2θ positions and FWHM are determined for all the different {hkl} planes and different tilt (Ψ) angles.